QR Iterations

Consider the iteration

$$\begin{array}{rcl} Q_i R_i & \leftarrow & A_i \\ A_{i+1} & \leftarrow & R_i Q_i \end{array}$$

Here we have first computed the QR factorization of A_i, and then reversed their product to form A_{i+1}. From $A_i = Q_i R_i$ we have $R_i = Q_i^T A_i$, and substituting that into $A_{i+1} = R_i Q_i$ gives

$$A_{i+1} = Q_i^T A_i Q_i$$

and thus the QR step is a similarity transformation!

If the eigenvalues of A are all real, then this iteration almost always converges to an upper triangular matrix T. In this limit, the eigenvalues of T (and hence A, right?) are $t_{11}, t_{22}, \ldots t_{nn}$. T is called a *Schur form* for A and the eigenvectors of T are *Schur vectors* of A. Every matrix is unitarily similar to an upper triangular matrix, and $T = Q^* A Q$ is called a *Schur decomposition* of A.

As it stands, this *QR iteration* requires $\mathrm{O}(n^3)$ flops per iteraton. We can reduce this by an order of magnitude by first reducing A to Hessenberg form $H_0 = Q^T A Q$. The following iteration preserves the Hessenberg form, and if we use a Householder (or Givens) QR factorization it requires only $\mathrm{O}(n^2)$ flops:

$$\begin{array}{rcl} Q_i R_i & \leftarrow & H_i \\ H_{i+1} & \leftarrow & R_i Q_i \end{array}$$

Notice that if a Hessenberg matrix H has $h_{k+1,k} = 0$, then the eigenproblem *decouples*: it is a block triangular matrix, and the eigenvalues of H are the union of the eigenvalues of the diagonal blocks (which are Hessenberg). A Hessenberg matrix for which none of the subdiagonal elements are zero is called *unreduced*.

Now if λ is an eigenvalue of an unreduced Hessenberg matrix H, then the QR factorization $QR = H - \lambda I$ will have $r_{nn} = 0$ (right?), and thus $H_{new} = RQ + \lambda I$ will have last row λe_n^T. So what? $H_{new} = Q^T H Q$ is a reduced Hessenberg matrix: we just decoupled λ! Now we don't usually know λ a priori, but we *can* speed convergence of the QR iterations by shifting H_i at each step by an approximate eigenvalue:

$$\begin{array}{rcl} Q_i R_i & \leftarrow & H_i - s_i I \\ H_{i+1} & \leftarrow & R_i Q_i + s_i I \end{array}$$

This iteration is one of the most used methods to compute the eigenvalues and eigenvectors of symmetric (or Hermitian) matrices. In this case, H is both upper and lower Hessenberg, (called *tridiagonal*) and has only real eigenvalues. Furthermore, the QR iteration in this case requires only $\mathrm{O}(n)$ flops.

For nonsymmetric matrices we still have to address complex eigenvalues and the added cost of complex arithmetic...